Supporting Information

Chromatographic property classification of narrowly distributed ZnS quantum dots

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CONTENT:

SI 1. Parameters for ICP-OES measurements

Table SI 1: Parameters used for ICP-OES analysis.

	Flow rate / ml min^{-1}
Sample	0.6
Plasma gas (Ar)	10,000
Atomizing gas (Ar)	600
Auxiliary gas (N_2)	200

SI 2. Interactions of NPs and stationary phase

The interactions between ZnS QDs and stationary phase materials (SPMs) play a decisive role for the success of chromatographic classification of NP by size. Therefore, we investigated the adhesion of ZnS QDs ($x_{1,3}$ = 1.8nm) on potential SPMs prior any chromatographic studies within the HPLC system using shaking experiments. Additionally, those studies allowed us to monitor the long-term stability of NPs against agglomeration while being in contact with SPMs. Figure SI 2_1 depicts the time-dependent normalized extinction of ZnS QDs at a wavelength of the extinction maximum of 259 nm ($E_{259\,nm}(t)$) for the adhesion experiments on SPM 1 and SPM 2. As can be seen in Figure SI 2_1, for both SPMs (SPM 1: black dots, SPM 2: blue squares), the normalized extinction of ZnS QDs stays almost constant over the whole experimental period of six days. The slight fluctuations can be explained by the experimental errors.

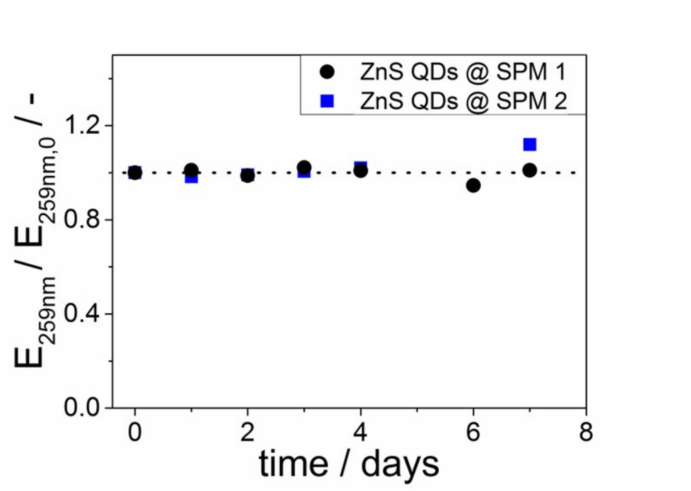

Figure SI 2_1: Normalized extinction at 259 nm over six days during shaking experiments of ZnS QDs ($x_{1,3}$ = 1.8 nm) in contact with SPM 1 particles (black dots) and SPM 2 particles (blue squares).

Therefore, no significant irreversible adhesion of ZnS QDs to both SPMs takes place. Hence, in general both materials would be suitable for the chromatographic separation of ZnS QDs. Noteworthy, the extinction spectra obtained in the adhesion experiments shown in Figure SI 2_2 also exclude any change in PSD due to agglomeration or ripening of the ZnS QDs. In this work and out of comparability reasons, we chose SPM 2 which we also used in our previous study on AuNPs. Thus, similar SPMs can be used for different types of particles and allow a direct comparison of the separation efficiency of ZnS QDs and AuNPs.

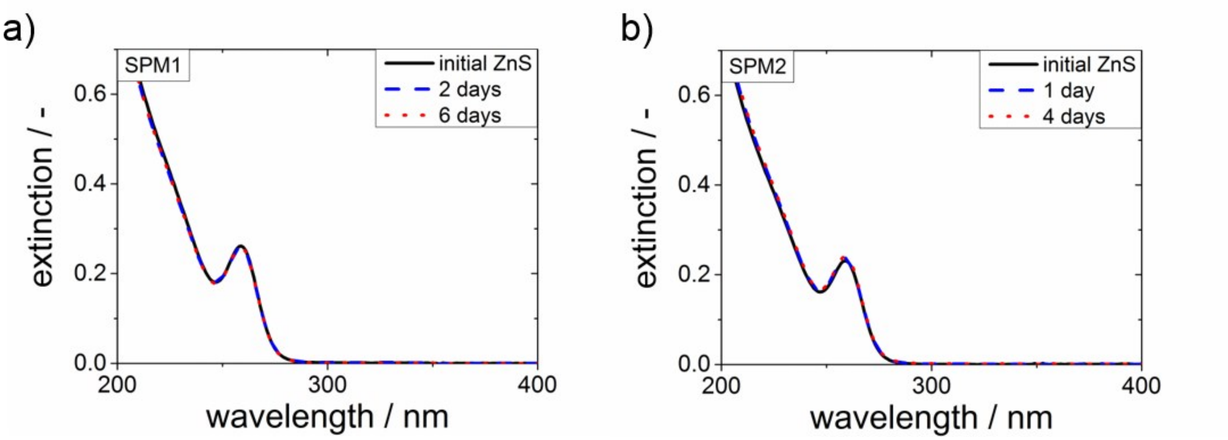

Figure SI 2_2: *Extinction spectra of ZnS QDs recorded during adhesion experiments using (a) stationary phase 1 and (b) stationary phase 2.*

SI 3. Normalized extinction spectra of ZnS QDs in Na_2HPO_4 buffer of different concentration before and after chromatographic experiment at different buffer concentration

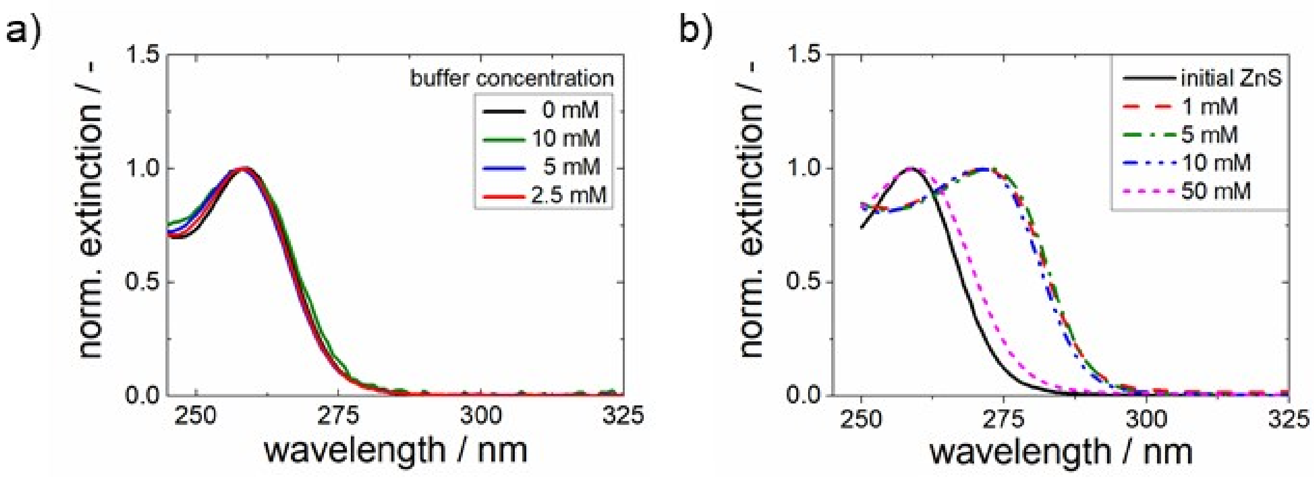

Figure SI 3: *Normalized extinction spectra of ZnS QDs ($x_{1,3}$ = 1.8 nm) a) before and b) after chromatographic experiment measured for different Na_2HPO_4 buffer concentrations between 1 and 50 mM at a flow rate of 1 ml min^{-1} using 20 µl* *injection volume. The complete retention peak was collected as one fraction using the fraction collector.*

SI 4. Extinction spectra of ZnS QDs of coarse and fine fraction for different switching times of the fraction collector

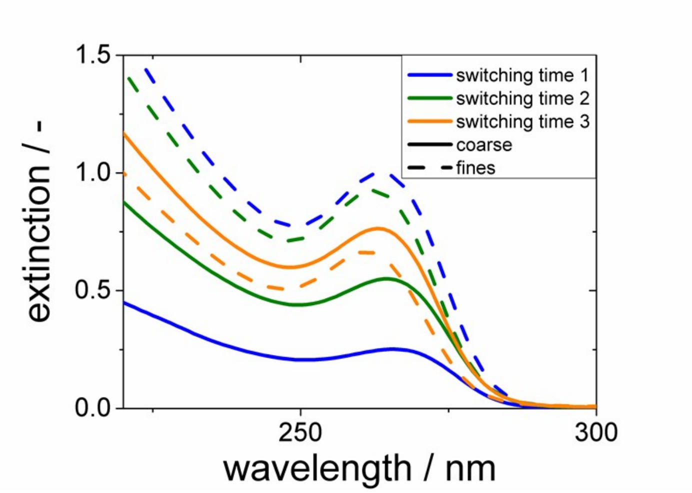

Figure SI 4: *Extinction spectra of obtained coarse and fine fractions after the chromatographic experiment for different switching times of the fraction collector (1:21.5 min; 1: 22.5 min; 3: 23.1 min) using a 50 mM* Na_2HPO_4 *buffer at a flow rate of 0.3 ml* min^{-1} *and a 20 µl injection volume and a detection wavelength of 250 nm.*

SI 5. Mass fractions for classification experiments with varying flow rate obtained by ICP-OES

Table SI 5: Obtained coarse and fine fractions for chromatographic experiments using the fraction collector.

	Switching at retention peak maximum	
Flow rate / ml min^{-1}	coarse	Fines
0.2	0.39	0.61
0.3	0.36	0.64
0.5	0.28	0.72
1.0	0.37	0.63

SI 6. Mass-weighted band gap distributions measured for ZnS QDs at different flow rates

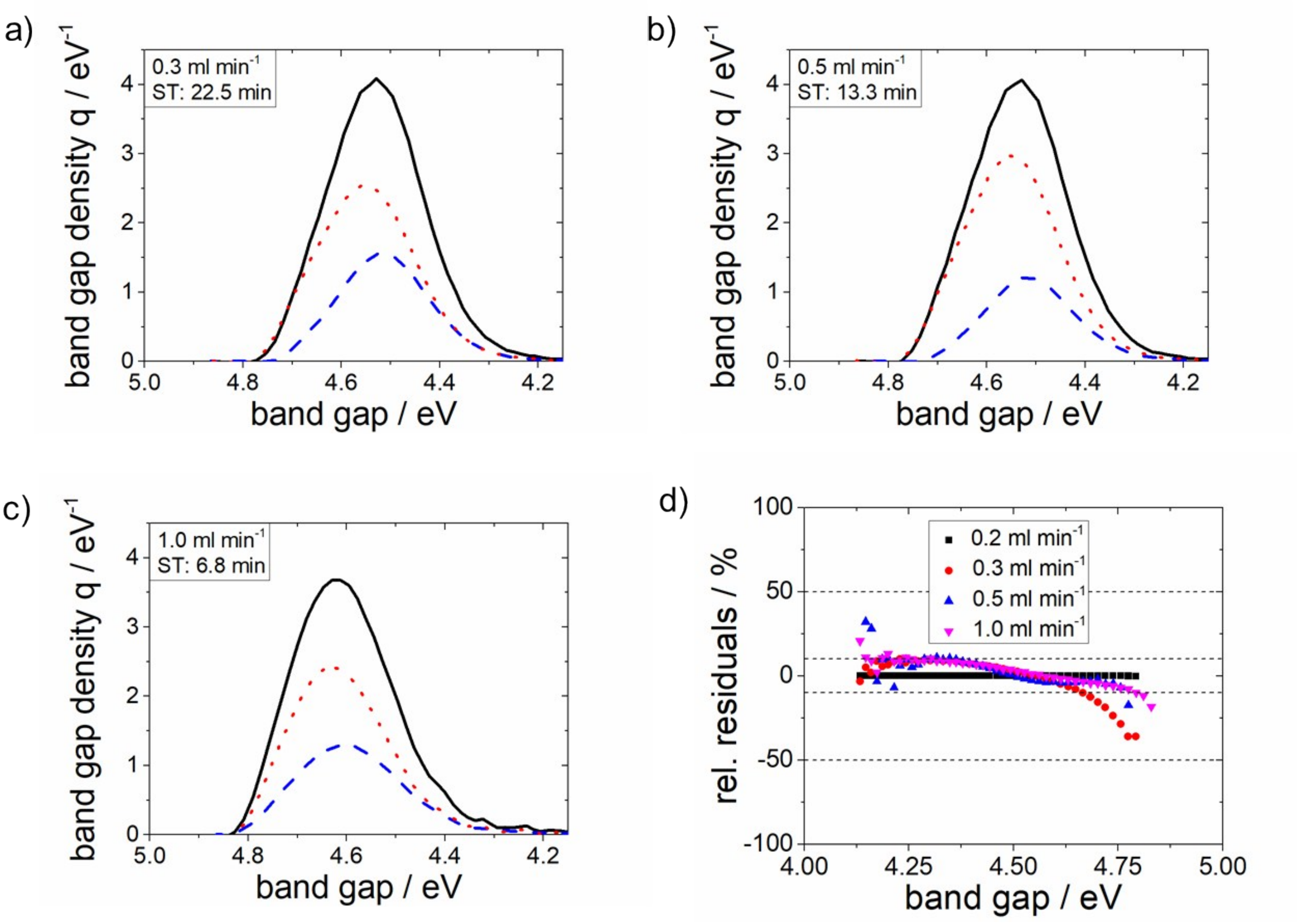

Figure SI 6: *Band gap distributions of feed ZnS QDs (black solid line) and mass-weighted band gap distributions of coarse (blue dashed line) and fines (red dotted line) for switching of the fraction collector in maximum of chromatogram at a flow rate of (a) 0.3 ml min^{-1}, (b) 0.5 ml min^{-1} and (c) 1.0 ml min^{-1}. (d) shows the residuals q(feed)-(g·q(coarse)+f·q(fines)) relative to q(feed) as a measure for the degree of fulfilling the mass balance. If the mass balance is perfectly* *fulfilled the residuals are 0. The horizontal dashed lines in (d) at ±10% and ±50%, respectively, are guides for the eye to get a faster impression of the order of magnitude of the relative residuals.*

SI 7. Mass fractions for classification experiments with varying switching times obtained by ICP-OES

Table SI 7: Obtained coarse and fine fractions at different STs for chromatographic experiments using the fraction collector.

	Switching time 21.5 min		Switching time 22.5 min		Switching time 23.1 min	
Flow rate / ml min^{-1}	coarse	fines	coarse	fines	coarse	fines
0.3	0.14	0.86	0.36	0.64	0.50	0.50

SI 8. Mass-weighted band gap distributions measured for ZnS QDs at different switching times

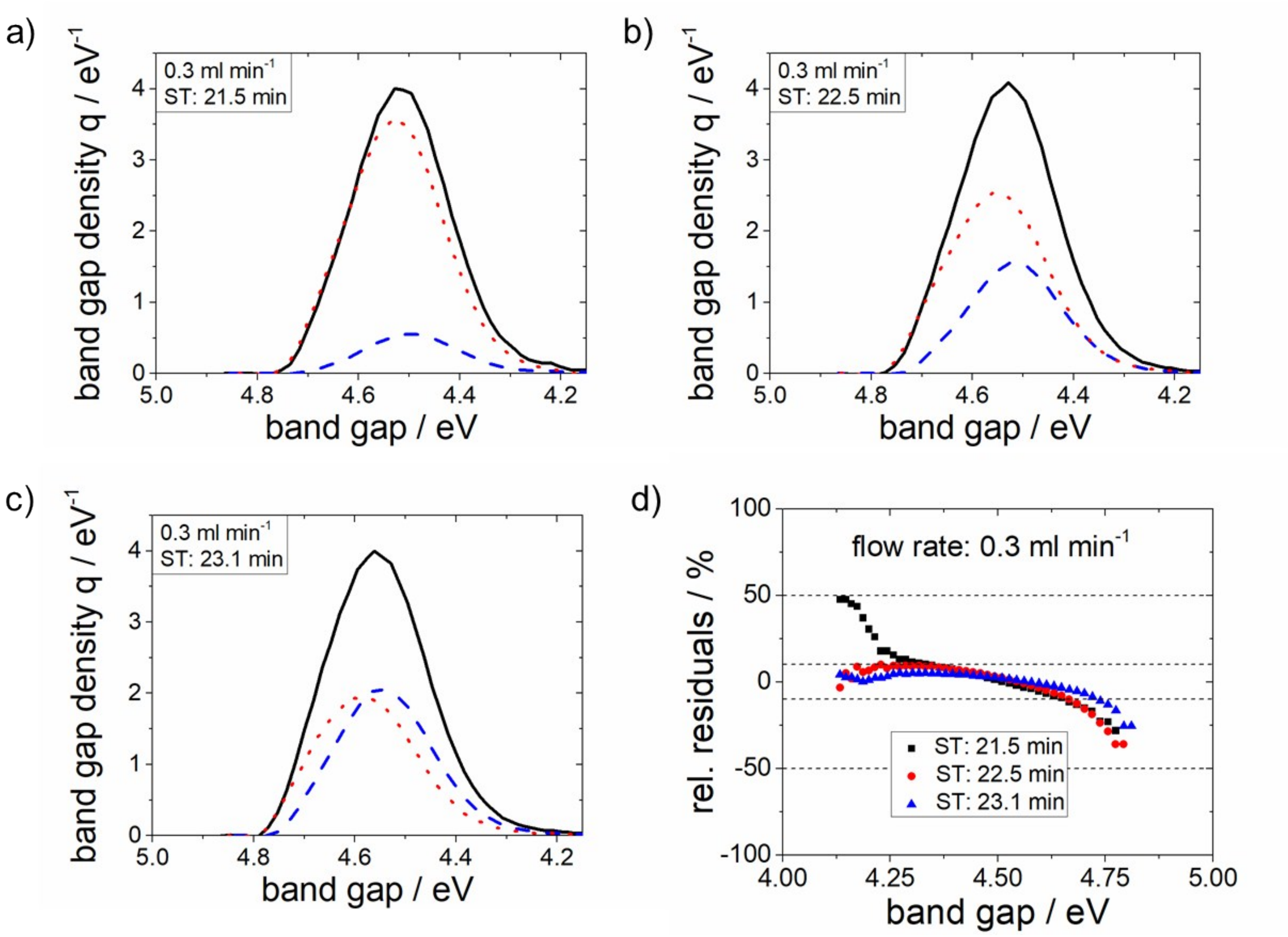

Figure SI 8: *Band gap distribution of feed ZnS QDs (black solid line) and mass-weighted band gap distribution of coarse (blue dashed line) and fines (red dotted line) at a flow rate of 0.3 ml min^{-1} for switching time (a) 21.5 min, (b) 22.5 min and (c) 23.1 min. (d) shows the residuals q(feed)-(g·q(coarse)+f·q(fines)) relative to q(feed) as a measure for the degree of fulfilling the mass balance. If the mass balance is perfectly fulfilled the residuals are 0. The horizontal dashed lines in* *(d) at ±10% and ±50%, respectively, are guides for the eye to get a faster impression of the order of magnitude of the relative residuals.*

SI 9. Mass fractions for classification experiments with varying temperature obtained by ICP-OES

Table SI 7: Obtained coarse and fine fractions at different STs for chromatographic experiments using the fraction collector.

	Temperature 7°C		Temperature 20°C		Temperature 40°C	
Flow rate / ml min^{-1}	coarse	fines	coarse	fines	coarse	fines
0.3	0.27	0.73	0.23	0.77	0.40	0.60

SI 10. Mass-weighted band gap distributions measured for ZnS QDs at different temperature

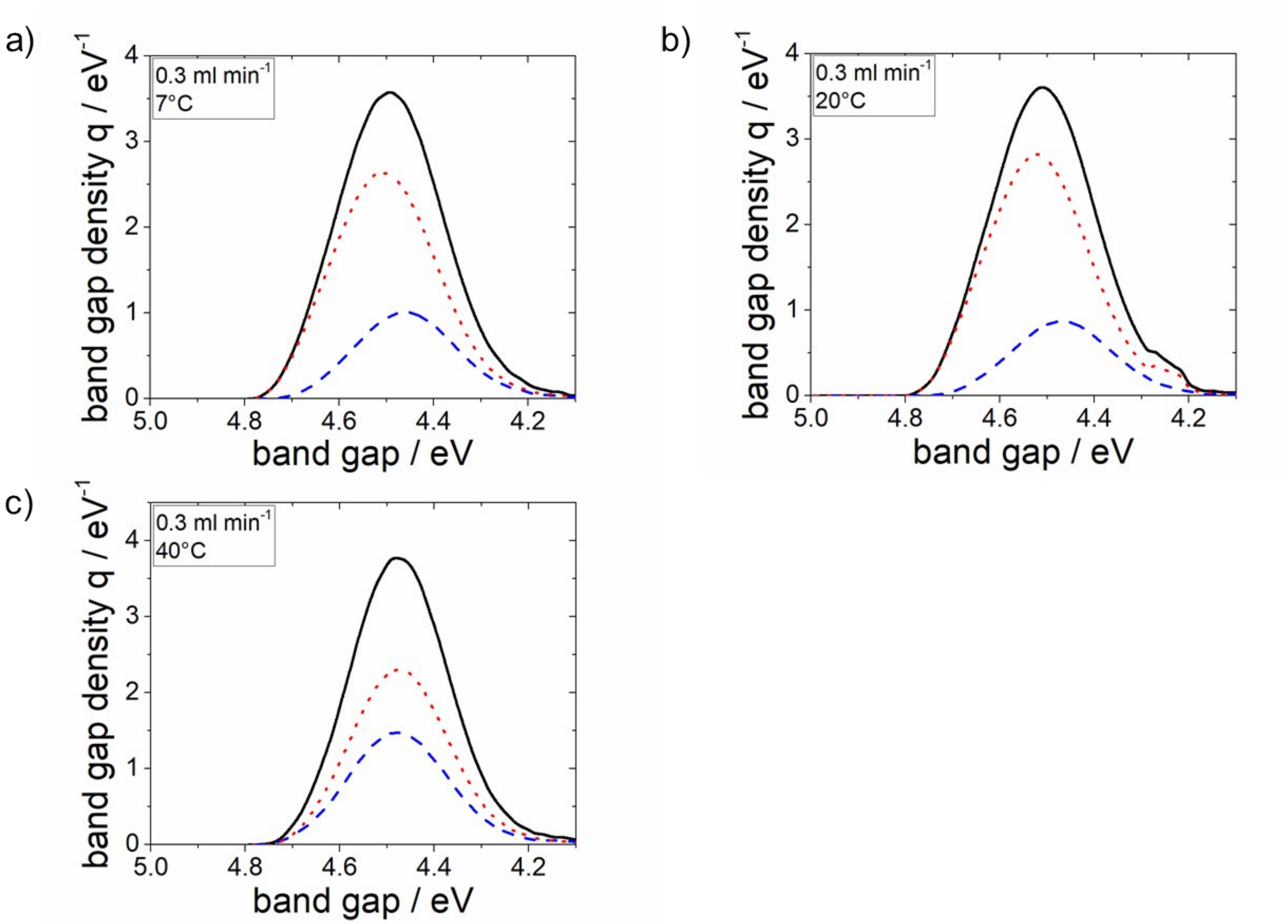

Figure SI 10: Band gap distribution of feed ZnS QDs (black solid line) and mass-weighted band gap distribution of coarse (blue dashed line) and fines (red dotted line) at a flow rate of 0.3 ml min^{-1} for temperature (a) 7°C, (b) 20°C and (c) 40°C. The switching time of the fraction collector was always set to retention peak maximum.

SI 11. FTIR spectrum of the ZnS QDs

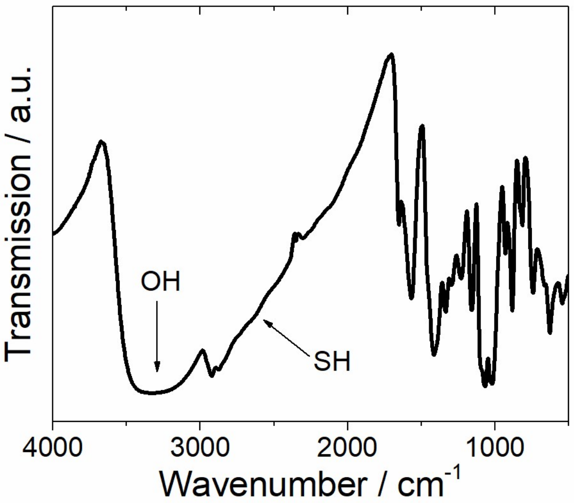

Figure SI 11: FTIR spectrum of the ZnS QD powder, the broad peak between 3500 and 2000 cm^{-1} indicates –OH and –SH stretch vibrations and thus, the presence of the capping agent 3-mercapto-1,2-propanediol (TG).

ABBREVIATIONS

ICP-OES	Inductively coupled plasma optical emission spectrometry
PSD	Particle size distribution
QDs	Quantum dots
SEC	Size-exclusion chromatography
SPM	Stationary phase material

SYMBOLS

Latin symbols

f	Relative mass of the fine fraction	-
g	Relative mass of the coarse fraction	-
q_f	Band gap distribution of the fine fraction	eV^{-1}
q_F	Band gap distribution of the feed	eV^{-1}
q_g	Band gap distribution of the coarse fraction	eV^{-1}